Simulations of "Decoherence" with Noise Pulses*

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A simulation of decoherence as random noise in the Hamiltonian is studied. The full Hamiltonian for the rf Squid is used, with the parameters chosen such that there is a double-potential well configuration where the two quasi-degenerate lowest levels are well separated from the rest. The results for these first two levels are in quantitative agreement with expectations from the "spin 1/2" picture for the behavior of a two-state system.

Back around 1980 Bob Harris and I wrote the first papers [1], [2] in the field which in the meantime has come to be called "decoherence ". My title should really be " Some Simulations of 'Quantum Damping' which is what Bobby and I called it in those days, but you can't fight MGM. Briefly, the message was–and is–that issues often thought to belong to the arcane domain of "measurement theory" could actually lead to effects of physical significance and could be calculated concretely.

We were trying to understanding why experiments we had proposed for the L↔R oscillations of chiral molecules [3] – still beautiful experiments waiting to be done— weren't as easy as they sounded. The enormous sensitivities theoretically possible were obviously too good to be true, but we wanted to understand the reason. The answer turned out to be "decoherence ".

The density matrix for a two-state system like (L,R) is a Hermitian 2x2 matrix, and since such a matrix can always be written in terms of the Pauli matrices σ we introduce three parameters $\mathbf{P}$ and write

$$\rho = 1/2(1 + \mathbf{P} \cdot \sigma) \; . \tag{1}$$

$\mathbf{P}$ may be looked at as a "polarization vector" in an abstract "spin space" and contains the information on the coherence of the two states. This language allows a helpful visualization as a "spin 1/2 system "–where the spin or polarization point of course in the abstract space–, and for the time development we study the motions of P. For this we have a "Bloch-like" equation

$$\dot{\mathbf{P}} = \mathbf{P} \times \mathbf{V} - D\,\mathbf{P}_T \; . \tag{2}$$

V represents the internal Hamiltonian and the damping parameter D the effects of the environment. D can change the length of P, while V cannot, and so for example can make a pure state ($|\mathbf{P}| = 1$) into a mixed state ($|\mathbf{P}| < 1$). Furthermore, as study of this equation shows, a large D inhibits the natural V-induced rotations of P, and so can stop or seriously slow down things like L↔R oscillations. Thus in addition to clarifying why the experiments aren't easy, "quantum damping" could also explain the permanence of optical isomers [4].

[The usual notation is such that the abstract "z-axis" corresponds to the property in question, so that $1/2(1+P_z)$ is the probability of finding L and $1/2(1-P_z)$ the probability of finding R. $\mathbf{P}_T$, where "T" stands for "transverse" means the components of $\mathbf{P}$ perpendicular to the "z- direction", that is the x,y components; it represents the degree of phase coherence between the two basis states. In Eq 2 we have taken the random external perturbations to be along the abstract z-axis, causing stochastic rotations around that axis. This corresponds to a low temperature situation where there is no direct barrier hopping between the two states.]

Given Eq 2, the important question becomes the calculation of D. We found a formula for it, resembling a kind of off-diagonal optical theorem, in terms of the S-matrices for the environmental atoms or molecules scattering on our system [1], [2]. However Bobby likes to understand things in more than one way and in the appendix to ref [1] he gave a little model in terms of random pulses rotating a spin.

Over the years this formalism has been generalized and applied in various fields [5]. Recently we have been working on the presently hot topic of mesoscopic devices and quantum computing, where for the latter subject decoherence is the major if not overriding issue. In particular we have gone into some detail for the rf Squid, showing for example how to perform the logic operations NOT and CNOT [6]. Thus we have been carrying out numerical simulations for these Squid-based systems, and recently we've begun to try simulating the effects of decoherence for the devices. This simulation is in some ways like the picture with random pulses in our old paper–a slightly fancier version with the pulses in the Hamiltonian, and I thought it might be amusing to present it here.

The rf Squid is described by a Hamiltonian where the "position coordinate" is ϕ, the flux in the Squid. In certain parameter ranges the potential in the Hamiltonian has a double-potential well form, as is shown in Fig 1.

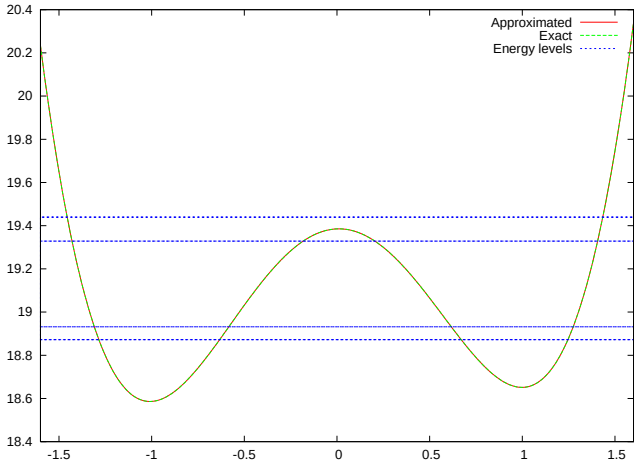

FIG. 1: An example of the potential in Eq 3 with ϕ^{ext}=0.0020. The first four energy levels from a numerical solution of the stationary Schroedinger equation are indicated. Varying ϕ^{ext}makes the potential asymmetric and allows manipulation of the levels and quantum gate operations.

The Hamiltonian is:

$$H = \frac{-1}{2\mu}\frac{\partial^2}{\partial\phi^2} + V_0\{\frac{1}{2}[(\phi - \phi^{ext})^2] + \beta\, cos\phi\} \; . \tag{3}$$

Fig 1 also shows the first four energy levels. The parameters μ, β and V_0 are related to the properties of the Squid. The quantity ϕ^{ext} is an external flux we can apply and vary to carry out our various operations, essentially it is used to raise and lower the relative heights of the two potential wells. We can adjust the parameters such that the two lowest states of this Hamiltonian, at ϕ^{ext}=0 split only by the small tunneling energy, effectively constitute a two-state system relatively well isolated from the other states of the Hamiltonian. Thus it should be describable by the formalism of Eqns 1,2, if we look only at the two lowest states.

We introduce decoherence into the system by supposing a random noise in the Hamiltonian and then evolving an initial wavefunction to a final wavefunction ψ^a with the Hamiltonian H^a with a given realization of the noise a. We then obtain the density matrix as an average over wavefunctions from different realizations

$$\rho = \overline{\psi\psi^\dagger} = \frac{1}{N}\sum_{a=1}^{N}\psi^a\psi^{a\dagger} \; . \tag{4}$$

The noise $\mathcal{N}$ is introduced into the Hamiltonian as a kind of flux noise–which may be physically the most relevant– by sending

$$\phi^{ext} \rightarrow \phi^{ext} + \mathcal{N}^a(t) \; , \tag{5}$$

so that for each realization of the noise $\mathcal{N}^a(t)$ we have some time dependent Hamiltonian H^a. This Hamiltonian is then used to evolve the wavefunction to obtain ψ^a.

In the computer the noise is generating by random pulses of magnitude $\pm\Delta$. The frequency of the noise is then governed by the effective time between sign switches. Analysis [8] of the effect of this in the Hamiltonian leads to the conclusion that for the effective two-state system composed of the two lowest states we should have

$$D = 4(V_0\phi_c)^2\int_0^\infty \overline{\mathcal{N}(t)\mathcal{N}(0)}dt = 4(V_0\phi_c)^2\frac{\Delta^2}{\omega_c} \; , \tag{6}$$

where ω_c is the frequency of the noise and ϕ_c is the "coordinate position" where the wavefunction tends to be localized, usually $\phi_c \approx 1$, as can be seen from Fig 1. The numerical evolution of the time dependent Schroedinger equation

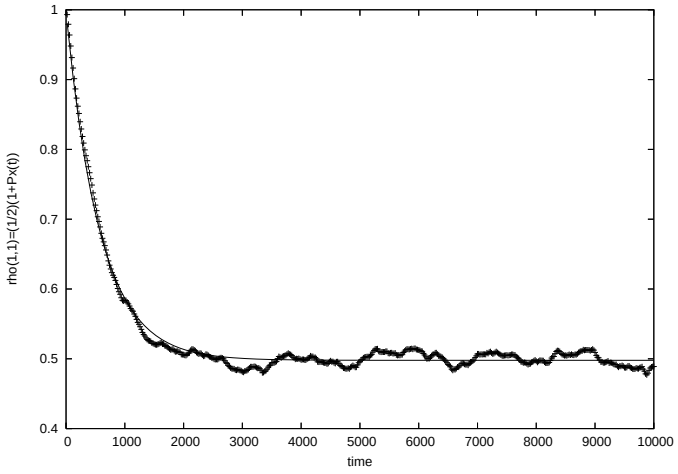

FIG. 2: Effect of decoherence as simulated with random noise in the Hamiltonian, with ϕ^{ext}=0. A pure state at t=0 is converted to the maximally mixed state for the two-state system. The exponential decay is e^{-Dt} is fit (thin line)with $D = 0.00175$, while the prediction from Eq 6 is D=0.00164. The quantity plotted is the probability of finding the original state, which is ρ_{11} in the basis of energy eigenstates or $(1/2)(1 + P_x)$. Noise parameters were $\Delta = 0.00032, \omega_c = .05$.

is carried out with a fast algorithm using algebraic manipulations in an harmonic oscillator basis [9]. The density matrix resulting from the average over wavefunctions $\psi^a(\phi)$ is then given in the "position coordinates" $\sim \rho(\phi', \phi)$. This is, however, not immediately in the form Eq 1. Although we hope that if we start in one of the two lowest states we stay there, we are now dealing with a many-state system, in principle containing components from all the states of the Squid Hamiltonian Eq 3. Therefore, depending on the question being asked, the results must be evaluated by finding the matrix elements of $\rho(\phi', \phi)$ in some basis of wavefunctions.

A first simple question we can ask is if we get the right behavior and the right D. For this purpose we can start with an energy eigenfunction of the symmetric ϕ^{ext}=0 Hamiltonian and examine the probability to find this state at a later time. The only energy splitting is due to the small tunneling (only $V_x \neq 0$) and the starting situation corresponds to **P** along the x-axis. Turning on the noise, we get Fig 2 for the evolution of the density matrix element for the probability of finding the initial state, that is $\rho_{1,1}$ in the basis of the original energy eigenstates, $\rho_{1,1} = (1/2)(1 + P_x)$. Gratifyingly, we see that ρ_{11} drops off exponentially to the value of 1/2, as Eq 2 would predict. Furthermore the value

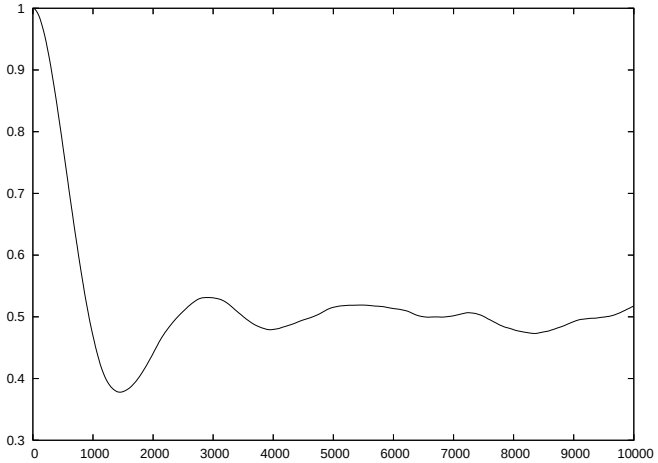

FIG. 3: Same conditions as Fig 2 but with the initial state in the "up" or "z- direction". Thus the vertical axis corresponds to $(1/2)(1 + P_z)$.

of D from the fit shown in the plot is D=0.00175, while the prediction from Eq 6 with the noise parameters used would be D= 0.00164. Also, although excitations of the higher states of the Squid were possible, the relaxation to 1/2 and not less shows that such excitations were small, at least for the parameters used here (they can be produced

by using large Δ). This and the good agreement with Eq 6 appears to show that, at least in this parameter range, the effective spin 1/2 picture using the first two states works well.

We can now try something a little more sophisticated with the same Hamiltonian, and start with an initial state where P points "up", that is in the abstract "z-direction". Since in this symmetric configuration the energy eigenstates "point" in the x-direction, this is no longer an energy eigenstate and in the absence of decoherence we would expect P to simply rotate in the z-y plane, around the x-axis. Fig 3 shows what happens, with the same parameters as for Fig 2. As would be expected, the oscillations and the damping combine to give damped oscillations. We hope to present more details and applications in the near future [8].

In conclusion I should perhaps stress that simulations such as these are only phenomenological and are not meant to replace calculations with the real basic physical amplitudes that determine D. For example, the phase [4], [7] arising in the full S- matrix treatment does not show up here. But of course the simulations can be quite useful in understanding what is to be expected for our logic gates. In any event our quantum damping is alive and well, and continues to find interesting and ever-widening applications.

The numerical work is based on the methods of J. Wosiek [9] as developed into a very useful program package by A. Görlich and P. Korcyl, students at the Jagellonian University, Cracow.

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